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Supplementary Material

A simple method for the analysis of neonicotinoids and their metabolites in human urine

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Table. S1 Liquid chromatography (LC) conditions and mass spectrometry (MS) parameters.

Table. S2 Mass transition of target analytes and internal standards. In each mass transition, 1: quantification ion, 2: confirmation ion.

Table. S1 Liquid chromatography (LC) conditions and mass spectrometry (MS) parameters.

Analyte	THX, IMI, ACE, THI, CLO, N-DMT, TA, IMZ, N-DMA			6-CN, SUF		
LC conditions						
Column	Betasil-C18 (3 μm, 100 × 2.1 mm)			Kinetex Phenyl/Hexyl (1.7 μm, 50 × 2.1 mm)		
Mobile phase A	Acetonitrile			Acetonitrile		
Mobile phase B	0.005% formic acid in water (v:v)			0.01% acetic acid in water (v:v)		
Flow rate (mL/min)	0.35			0.30		
Injection volume (μL)	3			3		
Gradients	Time (min)	A (%)	B (%)	Time (min)	A (%)	B (%)
	Initial	5	95	Initial	10	90
	1.2	5	95	0.5	10	90
	6.0	99	1	2.0	99	1
	8.0	99	1	3.8	99	1
	8.5	5	95	4.0	10	90
	10	5	95	5.0	10	90
MS conditions						
Ionization mode	ESI			ESI		
Polarity	Positive			Negative		
Curtain Gas	35			30		
Collision Gas	10			8		
IonSpray Voltage	4000			-4500		
Temperature	650			600		
Ion Source Gas 1	70			70		
Ion Source Gas 2	70			50		

Table. S2 Mass transition of target analytes and internal standards. In each mass transition, 1: quantification ion, 2: confirmation ion.

Positive	Compound	Precursor ion	Product ion	Internal standard	DP	EP	CE	CXP
	THX-1	291.8	211.1	$^{13}C_4$-^{15}N-THX-1	60	10	18	15
	THX-2	291.8	131.8	$^{13}C_4$-^{15}N-THX-2	60	10	27	15
	IMI-1	256	209	D_4-IMI-1	60	10	18	10
	IMI-2	256	175	D_4-IMI-2	60	10	30	10
	ACE-1	222.8	126	$^{13}C_6$-ACE-1	120	10	27	8
	ACE-2	222.8	90	$^{13}C_6$-ACE-2	120	10	39	10
	THI-1	253	126	$^{13}C_6$-THI-1	100	10	27	15
	THI-2	253	186	$^{13}C_6$-THI-2	100	10	21	10
	CLO-1	250	169.1	$^{13}C_3$-^{15}N-CLO-1	80	10	18	10
	CLO-2	250	131.9	$^{13}C_3$-^{15}N-CLO-2	80	10	21	15
	N-DMT-1	278	132	$^{13}C_4$-^{15}N-THX-1	60	10	21	15
	N-DMT-2	278	197.1	$^{13}C_4$-^{15}N-THX-2	60	10	18	10
	TA-1	271.1	126.1	$^{13}C_6$-THI-1	80	10	36	10
	TA-2	271.1	228.1	$^{13}C_6$-THI-2	80	10	20	15
	IMZ-1	262	181	D_4-IMI-1	80	10	21	10
	N-DMA-1	209	126	D_4-IMI-1	100	10	21	15
	N-DMA-2	209	90	D_4-IMI-1	100	10	40	10
	$^{13}C_6$-ACE-1	228.8	132	-	120	10	27	8
	$^{13}C_6$-ACE-2	228.8	96	-	120	10	39	10
	$^{13}C_6$-THI-1	259	132	-	100	10	27	15
	$^{13}C_6$-THI-2	259	192	-	100	10	21	10
	D_4-IMI-1	260	213	-	60	10	18	10
	D_4-IMI-2	260	179	-	60	10	30	10
	$^{13}C_3$-^{15}N-CLO-1	255	174.1	-	80	10	18	10
	$^{13}C_3$-^{15}N-CLO-2	255	136.9	-	80	10	21	15
	$^{13}C_4$-^{15}N-THX-1	296.8	216.1	-	60	10	18	15
	$^{13}C_4$-^{15}N-THX-2	296.8	136.8	-	60	10	27	15

Negative	Compound	Precursor ion	Product ion	Internal standard	DP	EP	CE	CXP	EX
	6-CN-1	155.9	111.9	$^{13}C_6$-6-CN-1	-35	-10	-15	-10	100
	6-CN-2	155.9	35	$^{13}C_6$-6-CN-2	-35	-10	-45	-8	100
	SUF-1	275.9	213	$^{13}C_3$-^{15}N-CLO	-80	-6	-21	-15	100
	SUF-2	275.9	170.9	$^{13}C_3$-^{15}N-CLO	-80	-6	-41	-20	100
	$^{13}C_6$-6-CN-1	161.9	116.9	-	-35	-10	-15	-10	100
	$^{13}C_6$-6-CN-2	161.9	35	-	-35	-10	-45	-8	100
	$^{13}C_3$-^{15}N-CLO	253	170	-	-80	-10	-23	-10	100